Towards the continuum limit in transport coefficient computations

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Abstract: The analytic continuation necessary for the extraction of transport coefficients is well-defined even in principle only when a continuous function of the Euclidean time variable is available. We report progress towards achieving the continuum limit for 2-point correlator measurements in pure SU(3) gauge theory, with specific attention paid to scale setting. As an application the determination of the heavy quark momentum diffusion coefficient from a correlator of colour-electric fields attached to a Polyakov loop is discussed.

I. Motivation

Among the most important quantities playing a role in the theoretical interpretation of heavy ion collision experiments at the LHC are so-called transport coefficients: shear and bulk viscosities as well as heavy and light quark diffusion coefficients. Because of strong interactions, these quantities need to be determined by lattice Monte Carlo simulations. This task is a hard one, given that numerical simulations are carried out in Euclidean signature, whereas transport coefficients are Minkowskian quantities, necessitating an analytic continuation (for a review see ref. [1]). Nevertheless, the problem is solvable in principle [2], provided that lattice simulations reach a continuum limit and short-distance singularities can be subtracted [3]. The purpose of this poster is to present progress in reaching the continuum limit with the example of a particular correlator.

II. Colour-electric correlator

Heavy quarks carry a colour charge and, whenever there are gauge fields present, are therefore subject to a coloured Lorentz force, which adjusts their velocities to those corresponding to kinetic equilibrium. Through linear response theory the effectiveness of the adjustment can be related to a "colour-electric correlator" [4,5],

$$G_{\rm E}(\tau) = -\frac{1}{3}\sum_{i=1}^{3}\frac{\left\langle \mathrm{Re\,Tr}\Big[U(\tfrac{1}{T},\tau)\, gE_i(\tau,\vec{0})\, U(\tau,0)\, gE_i(0,\vec{0})\Big]\right\rangle}{\left\langle \mathrm{Re\,Tr}[U(\tfrac{1}{T},0)]\right\rangle}$$

where gE_i denotes the colour-electric field, T the temperature, and $U(\tau_2,\tau_1)$ a Wilson line in the Euclidean time direction. A discretized version of this correlator is shown in **Fig. 1**.

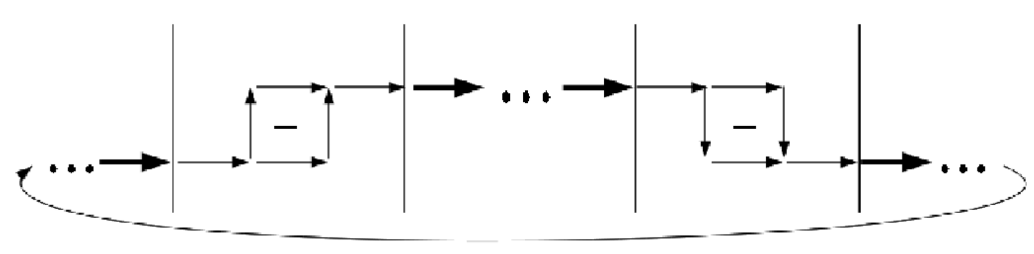

Fig. 1: Fat links, thin links and electric fields along the time direction.

If the spectral function corresponding to $G_{\rm E}(\tau)$, denoted by $\rho_{\rm E}(\omega)$, can be extracted (for a review see ref. [1]), then a "momentum diffusion coefficient", often denoted by κ, can be obtained from

$$\kappa = \lim_{\omega\to 0}\frac{2T\rho_{\rm E}(\omega)}{\omega}\,.$$

In the non-relativistic limit (i.e. for $M \gg \pi T$, where M stands for a heavy quark mass) the corresponding "diffusion coefficient" is given by $D = 2T^2/\kappa$.

We determine stochastic estimates for the function $G_{\rm E}(\tau)$ from large-scale simulations at a temperature $T \sim 1.42T_{\rm c}$ in pure gauge SU(3) lattice gauge theory. Box sizes substantially exceed those of earlier simulations [6,7,8], which had $V_{\rm max} = 24\times 64^3$. **Table 1** summarizes the situation with $N_{\rm conf}$ labelling the number of statistically independent configurations and $N_{\rm stat}$ the number of additional "multilevel" updates (see below).

β	N_τ	N_s	$N_{\rm conf}$	$N_{\rm stat}$	r_0T
6.872	16	32	140	1000	1.111
6.872	16	64	100	1000	1.111
7.192	24	96	160	1000	1.077
7.544	36	144	169	1000	1.068

Table 1: Run parameters. The values of r_0T are obtained through an interpolation/extrapolation as illustrated in **Fig. 4**. With the value of $r_0T_{\rm c}$ from **Fig. 4**, we have $T/T_{\rm c} = 1.42$ for $N_\tau = 36$.

III. Improved measurement

The correlator of **Fig. 1** is measured with the standard Wilson gauge action. For purposes of statistical error reduction we make use of two special techniques [7]: the "thick" links in-between the electric fields are handled through the Parisi-Pentronzio-Rapuano (PPR) link integration method [9,10], whereas the time intervals of width $3a$ enclosing the electric fields are subjected to $N_{\rm stat}$ extra updates with fixed boundary conditions in accordance with the multilevel philosophy [11]. The error reduction is illustrated in **Figs. 2a, 2b**.

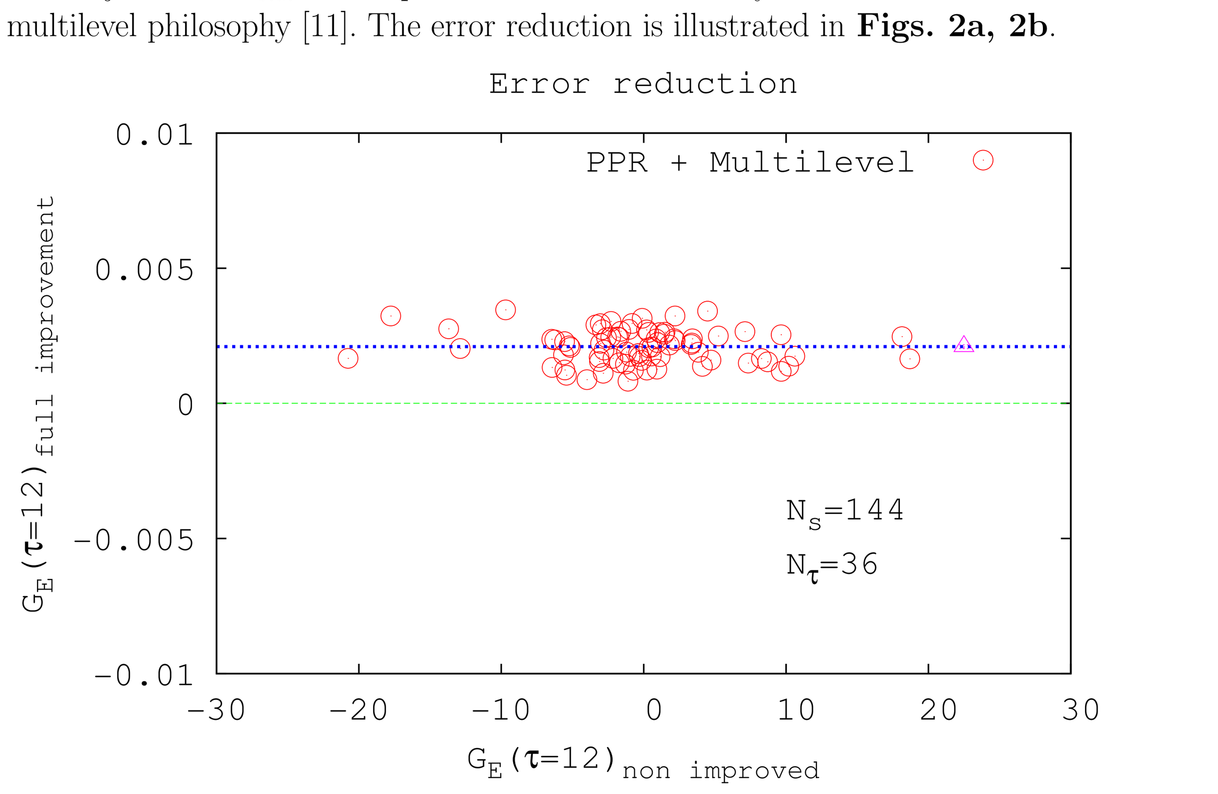

Fig. 2a: Error reduction for $G_{\rm E}(\tau = 12)$ in a 36×144^3 box. For 77 statistically independent configurations we determine the non-improved observable (x-axis) and the fully improved value (y-axis). A horizontal line and triangle mark the average of the improved observable.

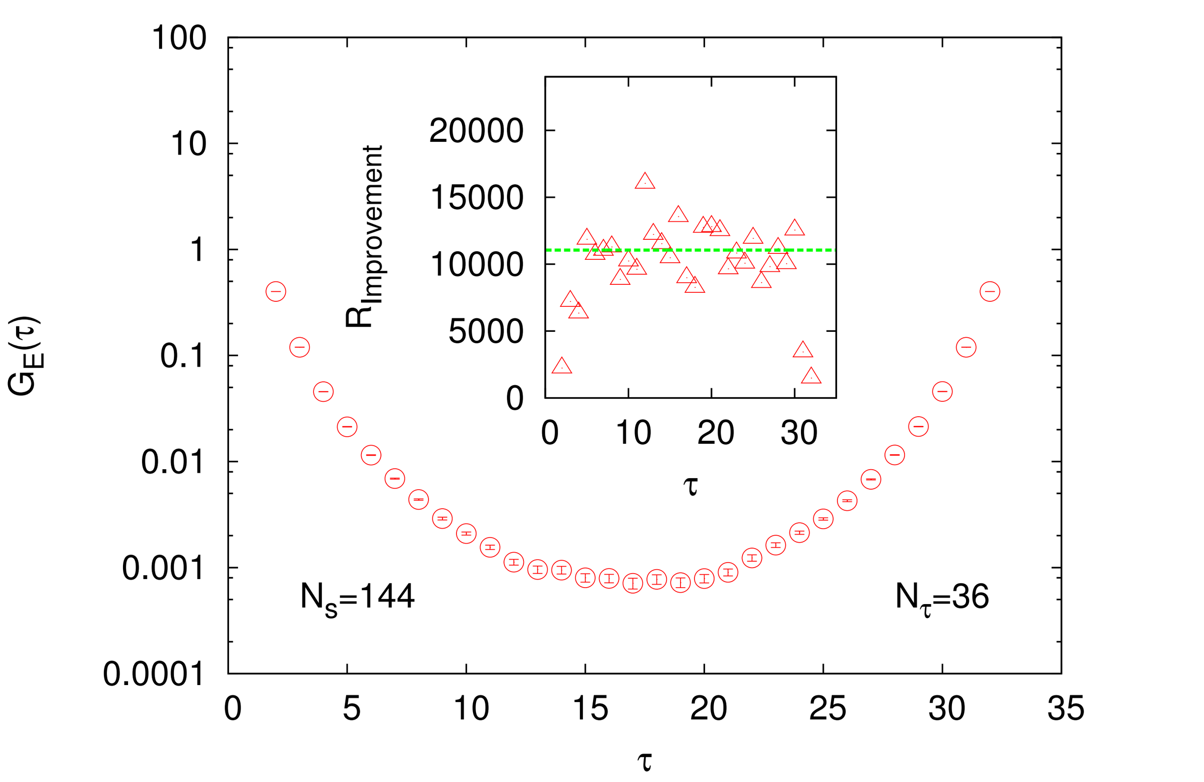

Fig. 2b: The improved correlator $G_{\rm E}(\tau)$. The inset shows the ratio of non-improved over improved statistical errors, denoted by $R_{\rm improvement}$. An error reduction by a factor $R^{-1}_{\rm improvement} \sim \mathcal{O}(10^{-4})$ can be achieved.

IV. Determination of the critical point

Pure SU(3) gauge theory possesses a first order phase transition at a certain $T_{\rm c}$. In order to express the results in a way that can be transported to full QCD, it is helpful to fix units in terms of $T_{\rm c}$. For a finite N_τ, this corresponds to a critical coupling $\beta_{\rm c}$. As a part of our investigation we have had another look at the classic problem of determining $\beta_{\rm c}$.

Because of computational limitations finite-temperature simulations with SU(3) Wilson action were historically carried out at small values of N_τ, say $N_\tau = 4-12$. Surprisingly, $\beta_{\rm c}$ has been determined reliably only in this range. (In addition to simulations, semi-analytic frameworks have been developed for estimating $\beta_{\rm c}$ [12,13], however these may contain uncontrolled uncertainties.)

We have carried out new simulations at $N_\tau = 12, 14, 16$, in each case with at least two spatial lattice sizes, denoted by N_s, in the range $N_s \geq 2N_\tau$. The critical point $\beta_{\rm c}$ is determined from the peak position of the susceptibility related to the Polyakov loop, and finite-size scaling in the inverse spacial volume $\propto N_s^{-3}$ is employed for extrapolating infinite-volume numbers. For illustration we display in **Fig. 3a** our Polyakov loop susceptibility data in a 14×40^3 box (at $N_s/N_\tau \approx 2.9$) and their corresponding Ferrenberg-Swendsen reweighting (denoted by the curve in the figure). Using the peak position of this data (the triangle) and a similar data set for a 14×56^3 box (at $N_s/N_\tau = 4$) a finite-size extrapolation gives $\beta_{\rm c}(N_\tau = 14) = 6.4501(14)$, with an error of less than one percent.

The curve in **Fig. 3b** displays also the result of lattice matching RG decimations [13]. Although our current estimate at $N_\tau = 16$ is preliminary ($\beta_{\rm c}(N_\tau = 16) \simeq 6.5537(46)$), it can be seen that the semi-analytic calculation misses some of the structure in the data.

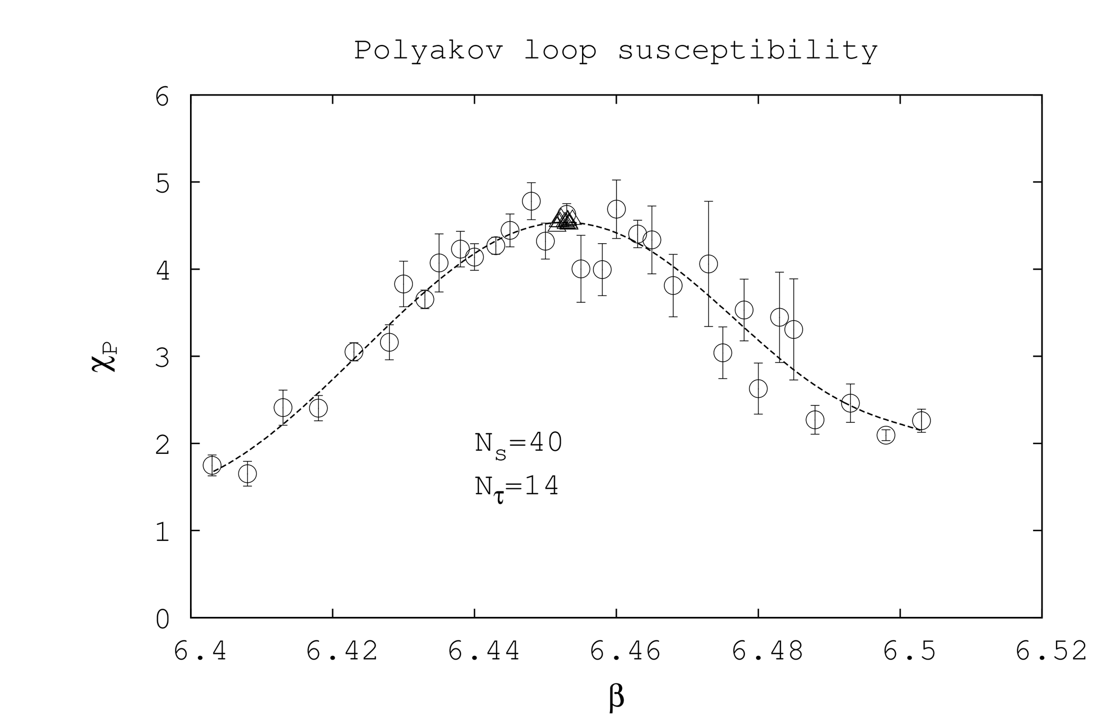

Fig. 3a: Polyakov loop susceptibility $\chi_{\rm P} \equiv V_{\rm space}(\langle P^2\rangle - \langle P\rangle^2)$ for a 14×40^3 box in pure SU(3) lattice gauge theory with the Wilson action.

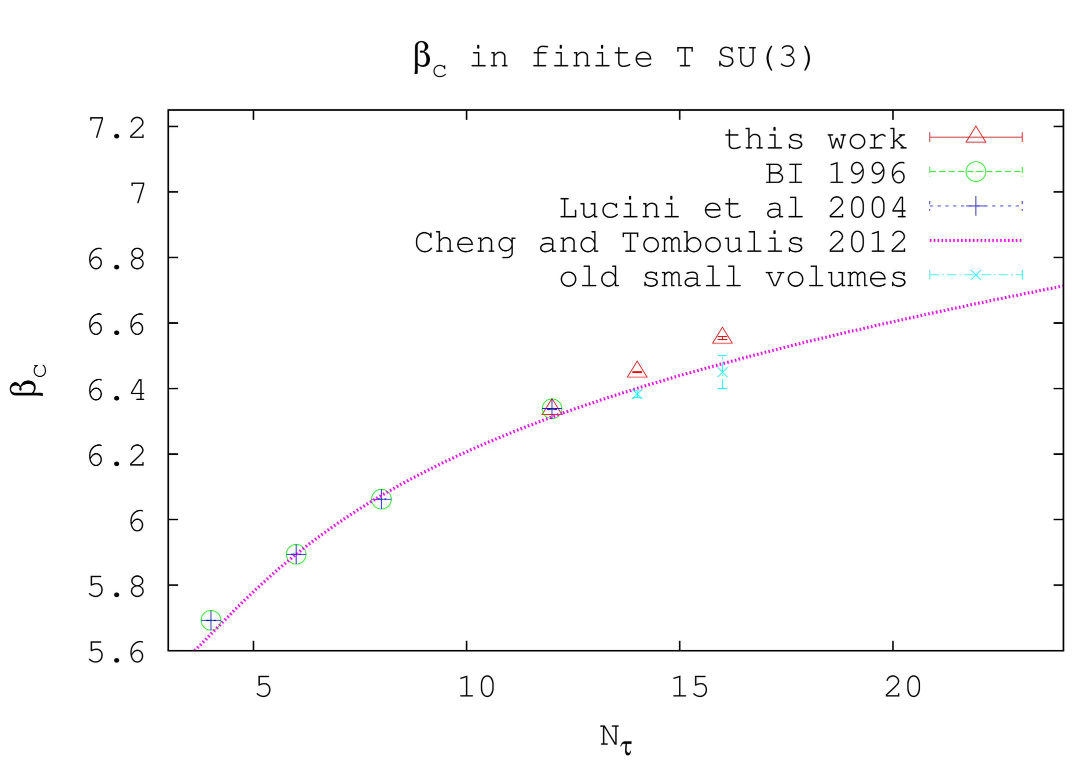

Fig. 3b: Published data for β_c, from Bielefeld (BI) [14] and Lucini et al [15], compared with our new data points at $N_\tau = 12, 14, 16$. The curve is an interpolation to the results of a semi-analytic study by Cheng and Tomboulis [13] (a semi-analytic study by Langelage et al can be found in ref. [12]).

V. Scale setting

A suitable auxiliary scale, allowing ultimately for a conversion of results to units of $T_{\rm c}$, is the Sommer scale r_0 [16]. The data of **Fig. 3b** can be used for determining $r_0T_{\rm c}$; the results are shown in **Fig. 4**. (We are currently also experimenting with another scale, introduced in ref. [17], which is based on Wilson flow and denoted by $\sqrt{t_0}$.)

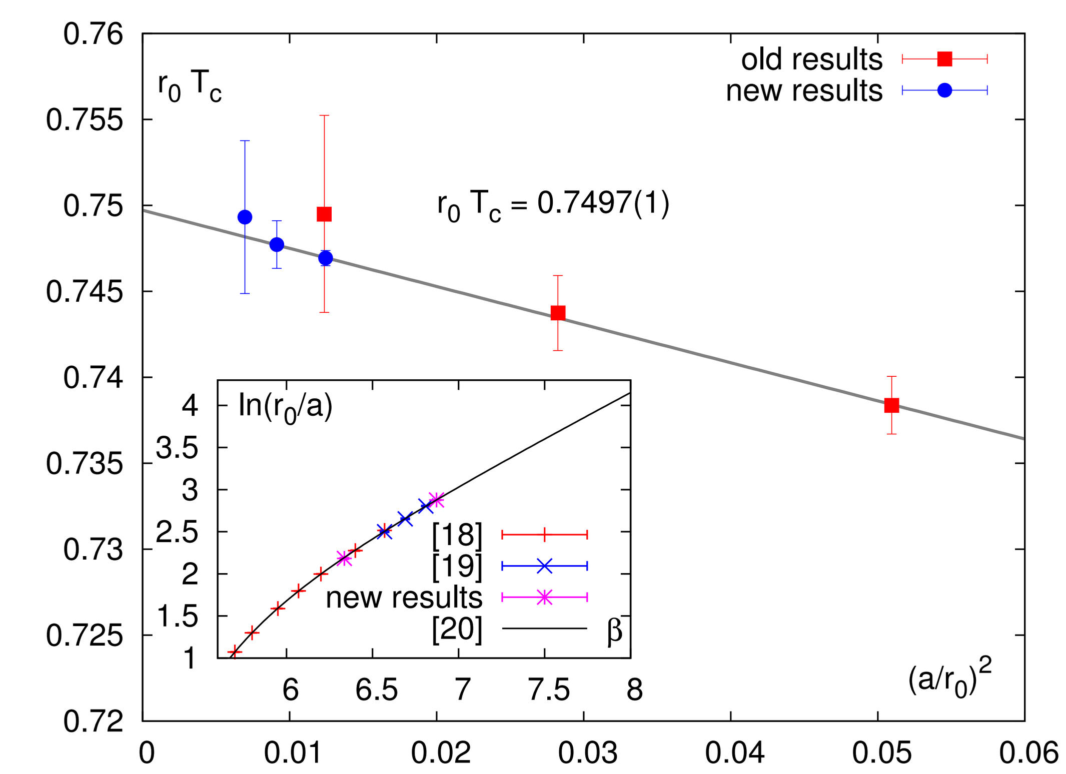

Fig. 4: Continuum extrapolation for $r_0T_{\rm c}$. The conversion from $\beta_{\rm c}$ to r_0/a is based on refs. [18,19] and additional new simulations, together with a rational interpolation from ref. [20] (inset). The result $r_0T_{\rm c} = 0.7497(1)$ can be contrasted with $r_0T_{\rm c} = 0.7498(50)$ from ref. [21]. (For comparisons with perturbation theory, $r_0\Lambda_{\overline{\rm MS}} = 0.602(48)$ from ref. [22] yields $T_{\rm c}/\Lambda_{\overline{\rm MS}} = 1.25(10)$; ref. [23] favours $r_0\Lambda_{\overline{\rm MS}} = 0.637(32)$ which yields $T_{\rm c}/\Lambda_{\overline{\rm MS}} = 1.18(6)$).

VI. Results for the correlator

After tree-level improvement [16,24] our measurements yield a correlator denoted by $G_{\rm imp}(\tau)$, which is furthermore multiplied by a perturbative renormalization factor $Z_{\rm pert}$ [7]. Normalizing the resulting correlator to

$$G_{\rm norm}(\tau T) \;\equiv\; \pi^2T^4\left[\frac{\cos^2(\pi\tau T)}{\sin^4(\pi\tau T)} + \frac{1}{3\sin^2(\pi\tau T)}\right]\,,$$

the data are displayed in **Fig. 5**. They exhibit a very clear non-perturbative enhancement over the next-to-leading order (NLO) prediction from ref. [25].

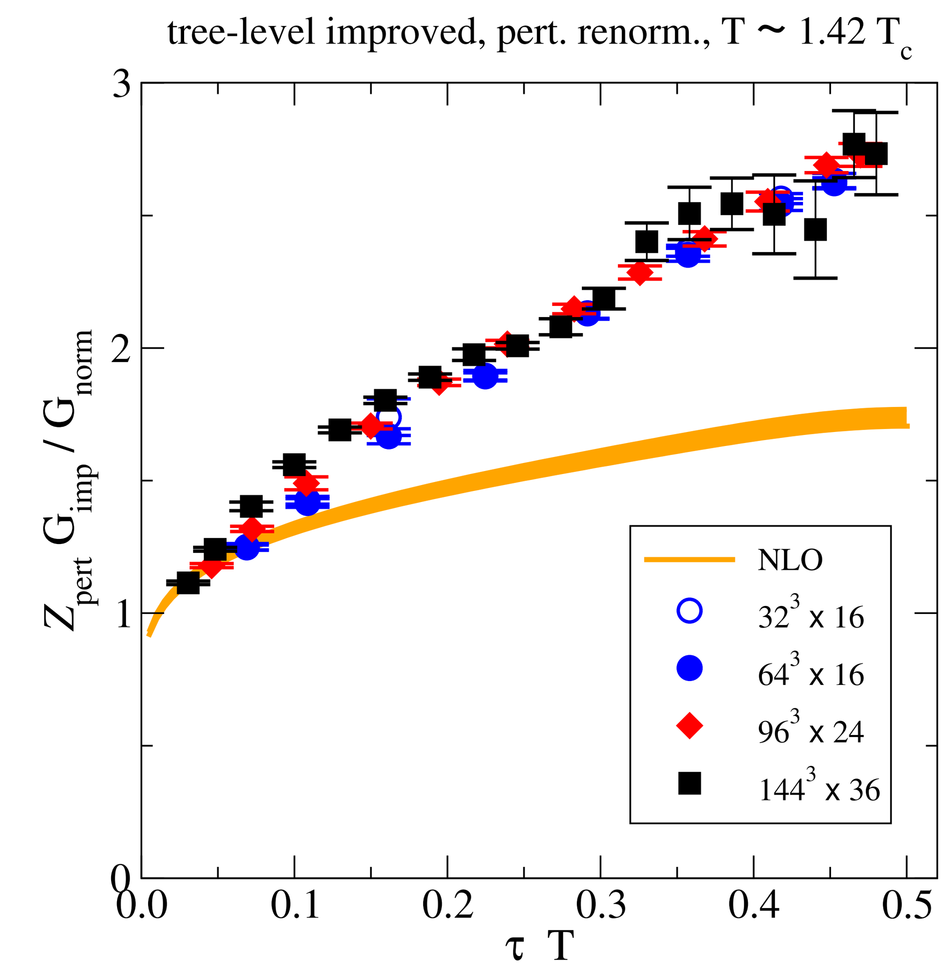

Fig. 5: Results for the colour-electric correlator at $T \sim 1.42T_{\rm c}$. For the NLO result we have varied $T_{\rm c}/\Lambda_{\overline{\rm MS}} \in (1.12, 1.35)$, cf. **Fig. 4**.

VII. Outlook

The Euclidean correlator is related to the spectral function $\rho_{\rm E}$ through

$$G_{\rm E}(\tau) = \int_0^\infty \frac{{\rm d}\omega}{\pi}\rho_{\rm E}(\omega)\frac{\cosh\left(\frac{1}{2}-\tau T\right)\frac{\omega}{T}}{\sinh\frac{\omega}{2T}}\,.$$

Our future goal is to combine the ingredients presented in this poster, in order to obtain a continuum extrapolation for $G_{\rm E}(\tau)$. Subsequently a perturbatively determined short-distance divergence may be subtracted, and the remainder subjected to an analytic continuation algorithm [2,3] or a well-motivated model like in refs. [7,8]. It will be interesting to see whether the preliminary values $D \sim (0.5\ldots0.8)/T$ [7,8] can be confirmed, and how well the results perform in phenomenological comparisons with LHC heavy ion data (cf. e.g. [26]).

VIII. References

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